

# Scale-free phase field theory of dislocations

István Groma,\* Zoltán Vándrus, and Péter Dusán Ispánovity

*Department of Materials Physics, Eötvös University Budapest, H-1517 Budapest POB 32, Hungary*

According to recent experimental and numerical investigations if the characteristic size of a specimen is in the submicron size regime several new interesting phenomena emerge during the deformation of the samples. Since in such a systems the boundaries play a crucial role, to model the plastic response of submicron sized crystals it is crucial to determine the dislocation distribution near the boundaries. In this paper a phase field type of continuum theory of the time evolution of an ensemble of parallel edge dislocations with identical Burgers vectors, corresponding to the dislocation geometry near boundaries, is presented. Since the dislocation-dislocation interaction is scale free ( $1/r$ ), apart from the average dislocation spacing the theory cannot contain any length scale parameter. As shown, the continuum theory suggested is able to recover the dislocation distribution near boundaries obtained by discrete dislocation dynamics simulations.

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Three dimensional crystals [1] and different 2D lattices, like Abrikosov vortices [2, 3], charge density waves [4, 5], or Wigner solids [6], generically contain a large number of line-type topological defects called dislocations greatly affecting the plastics response of these systems. Thus studying the collective properties of interacting dislocations is of utmost relevance in material physics. Although the interaction and dynamical properties of individual dislocations are well known for a long time, in most cases the deformation properties of the crystalline materials are controlled by the collective evolution of a large number of dislocations. One approach to model the rather complex phenomena caused by the collective motion of dislocations is the numerical solution of the equation of motion of individual dislocations called discrete dislocation dynamics (DDD). During the past decades numerous DDD simulation algorithms have been developed both in 2 [7–17] and 3 [18–22] dimensions, allowing to study problems like hardening [14, 18, 20], size effect [15, 21–24], jamming-flowing transition [10, 25], relaxation [17] dislocation avalanches [9, 16, 26], etc.

One may expect, however, that for a large number of problems not all the details accounted by DDD simulations are important, the response of the dislocation network can be well described on a continuum level. Although several such continuum theories of dislocations have been developed, [27–37] most of them correspond either to mean field approximation or are based on completely phenomenological grounds. However, the role of dislocation-dislocation correlation, crucial because of the long range nature of dislocation-dislocation interaction, is far from understood. Correlation effects are taken into account in a systematic manner only in the limit when the signed dislocation density  $\kappa$  (geometrically necessary dislocation (GND) density) is much smaller than the stored density  $\rho$ . [38–42].

With the advance of nanotechnology the characteristic size of the microstructure of crystalline materials reduced to the submicron level. As a consequence, the role

of boundaries (sample surface, grain boundary, etc.) has become even more important than earlier. So, to model the plastic response of samples with features on the submicron scale it is crucial to determine the dislocation distribution near the boundaries. Close to a boundary the GND density is often comparable to the stored one, so the assumption  $|\kappa| \ll \rho$  is not valid.

The dislocation distribution near a boundary is traditionally described by the 1D pile-up of the dislocations [43]. For many real dislocation configurations, however, the interaction between dislocations in different slip planes is important requiring to go up to modeling in minimum of 2D. In this paper a phase field type theory is suggested for the simplest possible 2D dislocation arrangement consisting of straight parallel dislocations with single slip. The evolution equations of the dislocation densities are obtained from a functional of the dislocation densities and the stress potential. In contrast to other approaches suggested recently, where a set of walls of dislocations with equidistant slip distances is considered to model the dislocation configuration near the boundary [34, 37], here we assume that the slip planes of the dislocations are arranged completely randomly. (In the present model dislocation climb is excluded, so the dislocations cannot leave their slip planes). Because of the  $1/r$ , *i.e.* scale-free, nature of dislocation-dislocation interaction, a key consequence of the random slip plane setup is that beside the coarse grained local dislocation spacing no other parameter with a length scale can appear in the theory. As it is explained in detail below this scale-free nature largely determines the possible form of the phase field potential. We speculate that the framework suggested could be applicable to other systems with scale free interaction, like gravitation.

Let us consider a system of parallel edge dislocations with line vectors  $\vec{l} = (0, 0, 1)$  and Burgers vectors  $\vec{b}_{\pm} = \pm(b, 0, 0)$ . The force in the slip plane acting on a dislocation is  $b\tau$  where  $\tau$  is the shear stress generated by the other dislocations plus the external shear. It is

commonly assumed that the velocity of a dislocation is proportional to the shear stress at the dislocation (over-damped dynamics) [39]. So, the equation of the motion of the  $i$ th dislocation positioned at point  $\vec{r}_i$  is

$$\frac{dx_i}{dt} = Mb\tau(\vec{r}_i) = Mb_i \left( \sum_{j=1, j \neq i}^N s_j \tau_{\text{ind}}(\vec{r}_i - \vec{r}_j) + \tau_{\text{ext}} \right) \quad (1)$$

where  $M$  is the dislocation mobility,  $\tau_{\text{ind}}$  is the stress field generated by a dislocation,  $\tau_{\text{ext}}$  is the external stress, and  $s_i = b_i/b = \pm 1$ . The coupled system of equations of motion can be solved numerically, that is called discrete dislocation dynamics (DDD) simulation.

As it was shown in detail in [40–42] the equation of motion of the dislocations Eq. (1) can be obtained from the variational “plastic” potential

$$P^d[\chi, \rho^d] = \int \left[ -\frac{D}{2} (\Delta \chi)^2 + b\chi \partial_y (\rho_+^d - \rho_-^d) \right] dx dy \quad (2)$$

as

$$\frac{\delta P^d}{\delta \chi} = -D \Delta^2 \chi + b \partial_y (\rho_+^d - \rho_-^d) = 0, \quad \dot{\vec{r}}_i = M \vec{b}_i \frac{\partial P^d}{\partial \vec{r}_i} \quad (3)$$

where  $D$  is a constant depending on the elastic moduli,  $\chi$  is the stress function with  $\tau = \partial_x \partial_y \chi$ , and  $\rho_{\pm}^d(\vec{r}) = \sum_{i=1}^{N_{\pm}} \delta(\vec{r} - \vec{r}_i)$  in which the summation has to be taken for the positive or negative signed dislocations, respectively. So,  $\rho_+^d(\vec{r})$  and  $\rho_-^d(\vec{r})$  are the “discrete” dislocation densities with the corresponding signs.

One may expect, however, that for many problems not all the details represented by the discrete description are needed. So, with appropriate coarse-graining one can obtain a continuum theory suitable to model the evolution of inhomogeneous dislocation systems. In order to derive a continuum theory from the “discrete” evolution equation, as a first step, one can replace in  $P^d$  given by Eq. (2) the “discrete”  $\rho_{\pm}^d$  fields by their local averages  $\rho_{\pm}$ , leading to the form

$$P_{\text{sc}}[\chi, \rho_{\pm}] = P^d[\chi, \rho_{\pm}]. \quad (4)$$

Although by applying the standard formalism of phase field theories, from  $P_{\text{sc}}$  one can derive evolution equations for the fields  $\rho_{\pm}$  in a systematic manner (see below), as it is explained in detail in [40, 41],  $P_{\text{sc}}$  corresponds to the mean (self-consistent) field approximation, i.e., dislocation-dislocation correlation effects are completely neglected. Due to the long-range nature of dislocation-dislocation interaction correlation effects are extremely important. So, terms accounting for correlations have to be added to  $P_{\text{sc}}$  to arrive at a physically relevant model.

As it is explained in detail in [40–42] because of the stress screening observed by DDD simulations for close to neutral systems ( $\kappa = \rho_+ - \rho_-$  is much smaller than  $\rho = \rho_+ + \rho_-$ ) correlations can be well accounted for by

adding a quadratic term in  $\kappa$  to  $P_{\text{sc}}$ . With this term, the potential reads as

$$P[\chi, \rho_{\pm}] = P_{\text{sc}}[\chi, \rho_{\pm}] + P_{\text{corr}}^{\pm}[\chi, \rho_{\pm}] \quad (5)$$

where

$$P_{\text{corr}}^{\pm}[\chi, \rho_{\pm}] = \int \frac{T_0}{2} \frac{\kappa^2}{\rho} dx dy, \quad (6)$$

in which  $T_0$  is a constant (with the dimension of force) determined by the dislocation-dislocation correlation function [41]. With the phase field formalism for conserved quantities the evolution equations for the fields  $\rho_{\pm}$  take the form

$$\dot{\rho}_{\pm} + \partial_x j_{\pm} = 0 \quad \text{with} \quad j_{\pm} = \mp M \rho_{\pm} \partial_x \frac{\delta P}{\delta \kappa}. \quad (7)$$

It should be mentioned that since the dislocation system is not a thermodynamical one there is no a priori reason that a phase field approach can be applied. So, the correctness of the above form has to be justified. Comparing it with the field equations obtained earlier [39] by a systematic coarse-graining procedure of the “discrete” system of evolution equations (3), one can see, that the phase field Eq. (7) is indeed justified if  $|\kappa|/\rho \ll 1$  [41].

For many configurations, like close to a grain boundary, however, the  $|\kappa|/\rho \ll 1$  condition, a key assumption in the microscopic derivation of the continuum theory, is not fulfilled. Therefore a new concept is needed to construct the correlation term. The primary aim of the present paper is to formulate a phase field theory if only one type of dislocation is present (say  $\rho_+$ ), representing the other extreme case  $|\kappa|/\rho = 1$ . (As it is discussed later, the general  $|\kappa|/\rho$  case can be established from the two extremes in a straightforward manner.)

Since  $P_{\text{sc}}[\chi, \rho_+]$  represents the mean field (i.e. correlationless) term, it is not affected by the  $|\kappa|/\rho$  ratio. The real nontrivial question is the possible form of  $P_{\text{corr}}[\chi, \rho_+]$  in this case. As a first possible approximation one can look for a term that does not contain the spatial derivatives of  $\rho_+$ . From simple dimensionality considerations the general form of such a term is

$$P_{\text{corr}}[\rho_+] = \int T \rho_+ f(\rho_+/\rho_0) dx dy, \quad (8)$$

where  $T$  is a constant,  $f(x)$  is an arbitrary function and  $\rho_0$  is a parameter with inverse length square dimension. For the following consideration a key point to notice is that since the dislocation-dislocation interaction is scale free, i.e. it does not contain any length scale parameter, the evolution equation of  $\rho_+$  also cannot contain any parameter with length dimension but the local dislocation spacing. As a consequence of this, the form of  $f(x)$  has to be chosen so that  $\rho_0$  does not appear in the phase field equation (7). To fulfill this condition the only possibility

is if  $f(x) \propto \ln(x)$ . With the above form of  $f(x)$  Eq. (7) takes the form

$$\dot{\rho}_+ + Mb\partial_x \left\{ \rho_+ \left[ \tau_{sc} - \frac{T}{b\rho_+} \partial_x \rho_+ \right] \right\} = 0, \quad \tau_{sc} = \partial_x \partial_y \chi \quad (9)$$

where  $\tau_{sc}$  is the “self consistent” or “mean field” shear stress. The evolution equation (9) has to be supplemented with appropriate boundary conditions. This depends on the actual properties of the boundaries, but it is quite a common case that the boundary is unpenetrable for the dislocations, so the dislocation current has to vanish at the boundaries if the Burgers vector is not parallel to the surface.

One can easily see, however, that the above “diffusive” like evolution equation is not satisfactory. Namely, let us consider a channel with surfaces perpendicular to the dislocation glide direction. After randomly placing dislocations with the same Burgers vectors into the channel and allowing the system to relax, a DDD simulation shows that the system does not remain homogeneous, boundary layers develop at the surfaces. A typical relaxed dislocation configuration obtained by DDD can be seen in Fig. 1, while the dislocation density obtained by averaging 5000 different realizations is plotted in Fig. 2.

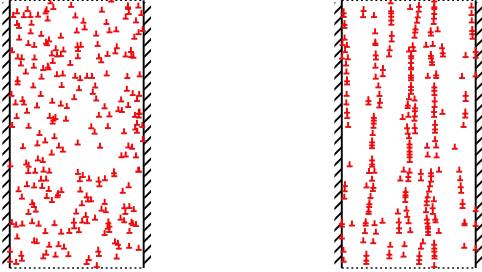


Figure 1: Random initial configuration of dislocations in a channel (left box). Relaxed dislocation configuration (right box). The walls are unpenetrable and periodic boundary condition is used in the  $y$  direction. The total number of dislocations is 256.

On the other hand, however, in case of zero external shear stress the homogeneous  $\rho_+$  is a stable solution of Eq. (9) obtained above. So one can conclude, Eq. (9) is not able to reproduce the dislocation configuration developing in a channel. As the form of  $P_{corr}$  is dictated by the scale free nature of dislocation-dislocation interaction, to resolve the discrepancy between the DDD simulation results and the prediction of Eq. (9) one has to introduce gradient terms in  $\rho_+$  into  $P_{corr}$ . Again, to avoid the appearance of length scale parameters in the evolution equation the possible form of  $P_{corr}$  depending on  $\nabla \rho_+$  is

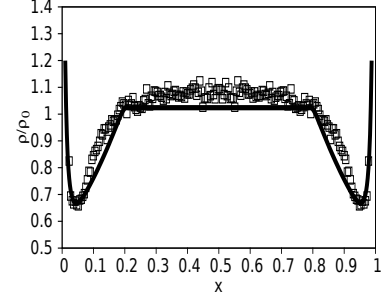


Figure 2: Dislocation density profile (relative to the initial density), averaged in the direction perpendicular to the slip direction, developing between two unpenetrable walls after the relaxation of an initially random system of dislocations with the same Burgers vectors obtained by DDD simulation (squares). The numerical solution of the phase field model proposed (full line). Relevant simulation parameters are:  $u=0.1$ ,  $W_x=5.5$ ,  $\alpha_m = 0.1$ .

$$P_{corr} = \int_D T\rho_+ \left[ \ln \left( \frac{\rho_+}{\rho_0} \right) + u \left( \frac{\nabla \rho_+ \hat{S} \nabla \rho_+}{2\rho_+^3} \right) \right] dx dy, \quad (10)$$

where  $\hat{S}$  is a symmetric dimensionless  $2 \times 2$  matrix and  $u(x)$  is an arbitrary function. If  $|\nabla \rho_+ / \rho_+^{3/2}| \ll 1$  one can take the leading linear term in  $u(x)$ , so  $P_{corr}$  used in the considerations below is quadratic in  $\nabla \rho_+$ .

Due to the gradient terms introduced in  $P_{corr}$  the phase field equation (7) is a fourth order partial differential equation in  $\vec{r}$ . In order to get unique solution further boundary conditions have to be introduced beside the one introduced earlier for the dislocation current  $\vec{j}_+$ . A dislocation wall developing next to a boundary has an extra surface energy which can be accounted for by adding a surface term to  $P_{corr}$ . For dimensionality reasons the surface energy density has to be proportional to  $\sqrt{\rho_+}$ , but as above, parameters with length scale should not be introduced in the evolution equation of the dislocations, so the only possible form of the surface ( $\partial D$ ) contribution to the potential  $P$  is

$$P_{sf}[\rho_+] = \oint_{\partial D} \alpha_{sf} T \sqrt{\rho_+} \vec{n} d\vec{A} \quad (11)$$

where the  $\vec{n} = \vec{b}/b$  term takes into account that in the surface energy only the surface projection perpendicular to the slip plane has contribution, and  $\alpha_{sf}$  is a constant. (One may consider an appropriate  $\nabla \rho_+$  dependence of  $\alpha_{sf}$  but in this paper only the leading term independent from  $\nabla \rho_+$  is taken.) Since the relaxation of the dislocation configuration next to the surface is expected to be much faster than in the bulk, the boundary condition can be obtained from the total plastic potential

$$P[\chi, \rho_+] = P_{sc}[\chi, \rho_+] + P_{corr}[\rho_+] + P_{sf}[\rho_+] \quad (12)$$

given by Eqs. (4,10,11) as

$$\left. \frac{\delta P}{\delta \rho_+} \right|_{\partial D} = \vec{W} \cdot \nabla \rho_+ - \rho_+^{3/2} \Big|_{\partial D} = 0 \quad (13)$$

where  $\vec{W}$  is a dimensionless constant 2D vector depending on  $\hat{S}$ ,  $\alpha_{sf}$  and the surface direction.

The system of Eqs. (7,13) together with the condition that  $j_+$  vanishes at the system surface, represent a closed set of equations with unique solution. As it is discussed below, however, it is not able to account for the dislocation density evolution obtained by DDD simulation for the channel problem mentioned above. Namely, for this geometry due to the translation symmetry in the  $y$  direction Eq. (7) has a steady state solution satisfying the condition

$$\frac{\delta P}{\delta \rho_+} = \mu_0, \quad (14)$$

where  $\mu_0$  is a parameter (analogous to the chemical potential) depending on the initial average dislocation density. After substituting the actual form of  $P[\chi, \rho_+]$  given by Eqs. (4,10,11) into Eq. (14) we arrive at a second order ordinary differential equation for the steady state  $\rho_+(x)$ . With the analysis of the structure of the equation one can find that within the channel the steady state solution is either completely convex or concave depending on the actual value of the parameters, i.e. it is not able to recover the shape seen in Fig. 2. even for a general  $u(x)$ . Another related issue is that according to DDD simulation results, the relaxed configuration of a dislocation system can vary if the initial dislocation density field is rearranged while the total number of dislocations (or average dislocation density) is kept constant. So, the steady state dislocation density does not reach always the same configuration represented by Eq. (14) at the same physical parameters.

To resolve the problem it is natural to assume that a system of dislocations with identical sign has an “internal rigidity” meaning that if the internal shear stress  $\tau_{int} = \partial_x(\delta P/\delta \rho_+) - \tau_{sc}$  is smaller than a critical value the system cannot rearrange itself. This is somewhat similar to the “flow stress” of neutral systems but for a single signed system the flow stress is obviously zero since under an external stress the whole system can move rigidly. Although the “internal rigidity” is a dislocation-dislocation correlation effect (like the flow stress introduced in [39] for neutral systems) there is no trivial way to take it into account by adding an appropriate term to  $P[\chi, \rho_+]$ . Within the phase field framework, however, it is possible to introduce a mobility function giving the dislocation current as

$$j_+ = Mb\rho_+ [M(\tau_{int}) + \tau_{sc}] \quad (15)$$

with

$$M(\tau) = \begin{cases} 0 & \text{if } \tau < \tau_0 \\ \tau - \tau_0 & \text{if } \tau > \tau_0 \end{cases} \quad (16)$$

Since there is no other length scale but the dislocation spacing, from a simple dimensionality consideration  $\tau_0 = \alpha_m b D^{-1} \sqrt{\rho_+}$ . The quantity  $\alpha_m$  may depend on the possible different dimensionless combinations of the dislocation density and its derivatives but in our analysis it was kept constant. An important consequence of this “critical type” mobility function is that the dislocation system cannot reach the configuration corresponding to the minimum condition given by Eq. (14).

As it is seen in Fig. 2 for the channel problem the numerical solution of the evolution equation with Eqs. (7,15,16) recovers the characteristic feature of the spatial variation of the dislocation density obtained by DDD.

Besides the channel problem discussed above it is interesting to analyze what happens with a localized dislocation density “peak” formed from dislocations with the same Burgers vector and homogeneous in the  $y$  direction. According to DDD simulation results, if one considers a dislocation density peak with random dislocation positions it starts to spread out but it reaches a steady state shape depending on the initial width and dislocation density. Without the gradient term in  $P_{corr}$  given by Eq. (10) and the nontrivial mobility function (16) the evolution equation would be a “diffusion” like equation predicting a complete spread out of the density peak. So, the main message of this paper is the non-diffusive behavior of the dislocation system.

According to the discussion explained above we have at hand continuum theories of dislocations in two extreme cases: if  $|\kappa/\rho| \ll 1$  and if  $|\kappa/\rho| = 1$ . It is natural to assume that the general  $\kappa/\rho$  case can be obtained by a smooth interpolation between the limits. (Since the mean field part of the plastic potential  $P_{sc}$  is valid for any  $\kappa$  we have to consider only the correlation part of  $P$ ). As a first step let us simply take the sum  $P_{corr}^t[\rho_+, \rho_-] = P_{corr}[\rho_+] + P_{corr}[\rho_-]$ . If  $|\kappa/\rho| \ll 1$  and we neglect the terms depending on the derivatives of the dislocation densities one obtains that  $P_{sc} + P_{corr}^t$  recovers the form of  $P$  given by Eq. (6) if  $T = T_0$ . Since, however,  $T$  and  $T_0$  are determined by the dislocation-dislocation correlation functions [40, 41] depending on the  $\kappa/\rho$  ratio, one cannot expect that  $T = T_0$ . It is useful to rewrite, however, the two logarithmic terms in  $P_{corr}^t$  into the form

$$T\rho_+ \ln(\rho_+/\rho_0) + T\rho_- \ln(\rho_-/\rho_0) = \frac{T}{2}\rho \ln \left[ \frac{\rho^2 - \kappa^2}{4\rho_0^2} \right] + \frac{T'}{2}\kappa \ln \left[ \frac{\rho + \kappa}{\rho - \kappa} \right] \quad (17)$$

(with  $T = T'$ ). For a general  $\kappa/\rho$  the coefficient  $T'$  can have a weak  $\kappa^2/\rho^2$  dependence in the form of  $T'(x) = T + (T_0 - T)(x - 1)^2/2$ . (Since in the evolution equations the functional derivative has to be taken only with respect to  $\kappa$ , term depending only on  $\rho$  can be dropped out from  $P_{corr}^t$ .) Two things that should be mentioned at this point: *i*) the  $\frac{dT'}{dx}(1) = 0$  condition ensures that no extra terms appears in  $\delta P/\delta \kappa$  at  $|\kappa| = \rho$  discussed above. *ii*)

the coefficient in front of the first term in the right hand side of Eq. (17) has to remain  $\kappa^2/\rho^2$  independent to ensure the  $\rho_0$  does not appear in the evolution equation of the dislocation densities. Without going into the details we mention a weak  $\kappa^2/\rho^2$  dependence of the coefficient in front of the gradient term in Eq. (10) can be introduced in a similar way. Certainly the actual values of the parameters appearing in the general form of  $P_{\text{corr}}$  have to be determined from DDD simulations corresponding to different system geometries.

In summary, a continuum theory of straight parallel dislocations is proposed that takes into account dislocation-dislocation correlation effects. The theory is obtained from a functional of the dislocation densities by applying the formalism of phase field theories. Although the phase field functional is established on a phenomenological ground, the actual form of the functional is largely dictated by the scale free nature of the dislocation-dislocation interaction. The theory is validated by comparing its predictions with DDD simulation. It has to be stressed that the form of the phase field functional proposed is the simplest possible one (containing only the leading order terms) that is able to recover the characteristic feature of the DDD simulation results. In order to recover the fine details of the DDD simulation results one may have to introduce higher order terms. Furthermore, certainly the 2D dislocation geometry the continuum theory is corresponding to is a strong simplification of the real much more complex 3D ones. In the 3D continuum theory, however, the structure of the terms corresponding to the correlation between dislocation loops should have rather similar forms.

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\* Electronic address: groma@metal.elte.hu

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